1,2-DODECANEDIOL

Other names: dodecane-1,2-diol
Inchi: InChI=1S/C12H26O2/c1-2-3-4-5-6-7-8-9-10-12(14)11-13/h12-14H,2-11H2,1H3
InchiKey: ZITKDVFRMRXIJQ-UHFFFAOYSA-N
Formula: C12H26O2
SMILES: CCCCCCCCCCC(O)CO
Mol. weight [g/mol]: 202.34
CAS: 1119-87-5

Physical Properties

Property code	Value	Unit	Source
af	0.9444		Cheméo Relay (1.0)
gf	-225.92	kJ/mol	Joback Method
hf	-605.19	kJ/mol	Cheméo Relay (1.0)
hfus	31.49	kJ/mol	Joback Method
hvap	111.61	kJ/mol	Cheméo Relay (1.0)
ie	10.01	eV	Cheméo Relay (1.0)
log10ws	-3.44		Cheméo Relay (1.0)
logp	2.870		Crippen Method
mcvol	191.680	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1621.00		NIST Webbook
rinpol	1621.00		NIST Webbook
tb	578.75	K	Cheméo Relay (1.0)
tc	755.86	K	Cheméo Relay (1.0)
tf	333.65 ± 0.40	K	NIST Webbook
tf	332.15 ± 2.00	K	NIST Webbook
vc	0.737	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.97	J/mol×K	657.88	Joback Method
cpg	558.13	J/mol×K	684.67	Joback Method
cpg	570.73	J/mol×K	711.47	Joback Method

cpg	582.81	J/mol×K	738.26	Joback Method
cpg	594.36	J/mol×K	765.05	Joback Method
cpg	605.42	J/mol×K	791.85	Joback Method
cpg	616.00	J/mol×K	818.64	Joback Method
dvisc	0.0247073	Pa×s	331.64	Joback Method
dvisc	0.0030604	Pa×s	386.01	Joback Method
dvisc	0.0006349	Pa×s	440.39	Joback Method
dvisc	0.0001861	Pa×s	494.76	Joback Method
dvisc	0.0000696	Pa×s	549.13	Joback Method
dvisc	0.0000310	Pa×s	603.51	Joback Method
dvisc	0.0000158	Pa×s	657.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.95107e+01
Coeff. B	-6.71291e+03
Coeff. C	-1.02710e+02
Temperature range (K), min.	451.92
Temperature range (K), max.	575.48

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119875&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume